

Regression Coefficient Example

This example shows how to compute regression coefficient matrices for Classical Least Squares (CLS), Principal Component Regression (PCR), and Partial Least Squares (PLS).

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Supporting Information

A Practical Guide to Chemometric Analysis of Optical Spectroscopic Data

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Compute Regression Coefficients

```
clearvars
load pnnl_napalm_data
```

Compute the regression coefficient matrices, B , for Classical Least Squares (CLS), Principal Component Regression (PCR), and Partial Least Squares (PLS).

```
[C_cls, B_cls] = pnnl_cls(A_train, C_train, A_unknown);
```

For PCR, use 3 principal components.

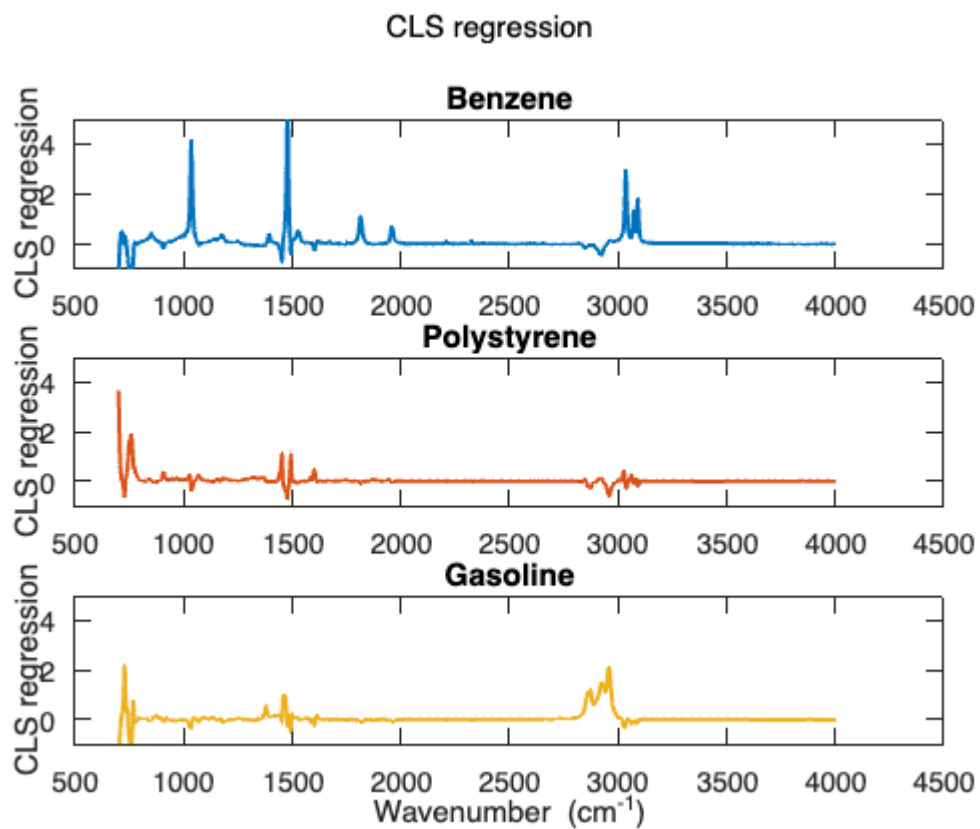
```
[C_pcr, B_pcr] = pnnl_pcr(A_train, C_train, A_unknown, 3);
```

For PLS, use 3 latent variables.

```
[C_pls, B_pls] = pnnl_pls(A_train, C_train, A_unknown, 3);
```

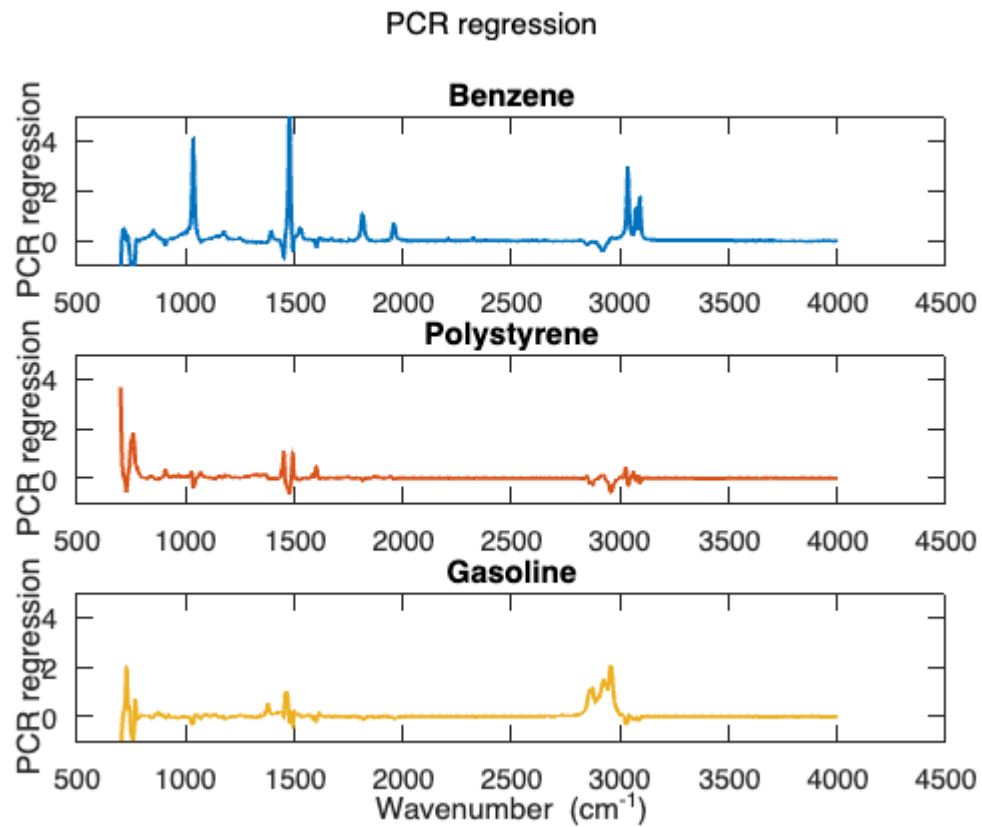
Plot regression coefficients for CLS.

```
plot_regression_coefficients(B_cls, 'CLS  
regression', Wavenumbers, WavenumberLabel, ConstituentNames)
```



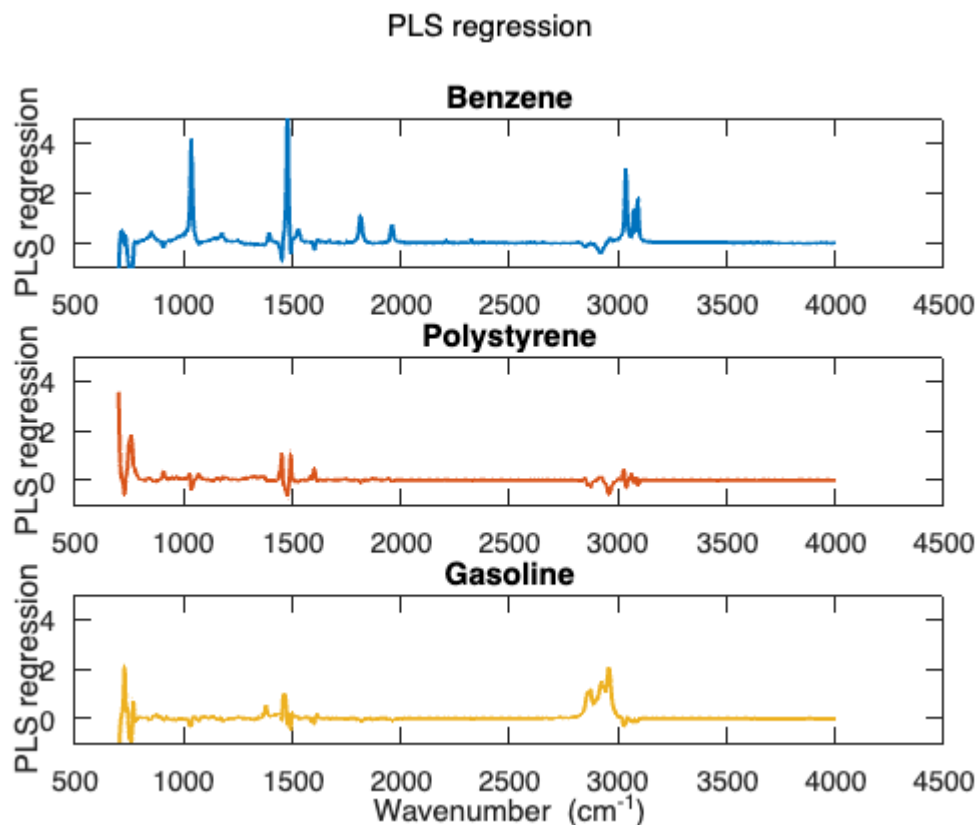
Plot regression coefficients for PCR.

```
plot_regression_coefficients(B_pcr, 'PCR  
regression', Wavenumbers, WavenumberLabel, ConstituentNames)
```



Plot regression coefficients for PLS.

```
plot_regression_coefficients(B_pls, 'PLS  
regression', Wavenumbers, WavenumberLabel, ConstituentNames)
```



```
function
plot_regression_coefficients(B,y_label,Wavenumbers,WavenumberLabel,ConstituentNames)
    figure
    n = size(B,2);
    colorOrder = pnnl_colorOrder(n);
    figure;
    h = gobjects(1,n);
    for j = 1:n
        h(j) = subplot(n,1,j);
        plot(Wavenumbers,B(:,j),'LineWidth',2,'Color',colorOrder(j,:));
        title(ConstituentNames{j})
        ylabel(y_label)
    end
    sgtitle(y_label)
    linkaxes(h)
    xlabel(WavenumberLabel)
    set(h,'FontSize',14,'YLim',[-1 5]);
end
```

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